26163-08-6 | DTXSID10737557

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 3500 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.44e-01

Confidence level: 7.81e-01

Nearest Neighbors from the Training Set

Image not found

Dimethyl sulfide
Measured: 5410
Predicted: 225

Image not found

Chrysene
Measured: 1170
Predicted: 1.80e-08

Image not found

Butane
Measured: 2250
Predicted: 1310

Image not found

1-Propene
Measured: 2310
Predicted: 4460

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Propoxur
Measured: 8690
Predicted: 6.68e-06